Direct Monte Carlo Simulation Of Chemical Reaction Systems

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Tutorial-7: Monte Carlo Simulations Monte Carlo Simulation

A Book for the Monte Carlo Method with Engineering Applications *Direct Monte Carlo Simulation Of*

Direct Simulation Monte Carlo (DSMC) method uses probabilistic (Monte Carlo) simulation to solve the Boltzmann equation for finite Knudsen number fluid flows. The DSMC method was proposed by Prof. Graeme Bird, Emeritus Professor of Aeronautics, University of Sydney. DSMC is a numerical method for modeling rarefied gas flows, in which the mean free path of a molecule is of the same order (or greater) than a representative physical length scale (i.e. the Knudsen number Kn is greater than 1).

Direct simulation Monte Carlo - Wikipedia

• Direct simulation Monte Carlo (DSMC) method is the Monte Carlo method for simulation of dilute gas flows on molecular level, i.e. on the level of individual molecules. To date DSMC is the basic numerical method in the kinetic theory of

gases and rarefied gas dynamics.

Direct Simulation Monte Carlo (DSMC) of gas flows
The simulation of e-beam scattering in structure implemented Direct Monte-Carlo (DMC) algorithm with discrete energy loss model . Elastic electron scattering in PMMA and Si was simulated using Mott elastic differential cross-sections , while different models were applied for inelastic process in PMMA and Si.

Direct Monte-Carlo simulation of dry e-beam etching of ...
In this work, direct simulation Monte Carlo computations have been performed to investigate flow separation and reattachment in a low-density hypersonic flow over such a configuration. Distinct features of leading-edge flow, limited boundary layer growth, separation, shear layer, flow structure in the recirculation region and reattachment are all explained in detail.

Direct simulation Monte Carlo computations and experiments ...
Monte Carlo Simulation, also known as the Monte Carlo Method or a multiple probability simulation, is a mathematical technique, which is used to estimate the possible outcomes of an uncertain event. The Monte Carlo Method was invented by John von Neumann and Stanislaw Ulam during World War II to improve decision making under uncertain conditions. It was named after a well-known casino town, called Monaco, since the element of chance is core to the modeling approach, similar to a game of ...

What is Monte Carlo Simulation? | IBM
Monte Carlo simulation and Navier – Stokes finite difference calculation of unsteady-state rarefied gas flows Physics of Fluids, Vol. 10, No. 1 DIRECT SIMULATION MONTE CARLO: Recent Advances and Applications Annual Review of Fluid Mechanics, Vol. 30, No. 1

Direct simulation Monte Carlo and Navier-Stokes ...
We propose a continuous-time formulation of the direct simulation Monte Carlo that allows the evaluation of the transport coefficient dependence on the time step through the use of the Green – Kubo theory. Our results indicate that the error exhibits quadratic dependence on the time step, and that for time steps of the order of one mean free time the error is of the order of 5%.

Analysis of discretization in the direct simulation Monte ...
SPARTA is an acronym for Stochastic PArallel Rarefied-gas Time-accurate Analyzer. SPARTA is a parallel DSMC or Direct Simulation Montel Carlo code for performing simulations of low-density gases in 2d or 3d. Particles advect through a hierarchical Cartesian grid that overlays the simulation box. The grid is used to group particles by grid cell for purposes of performing collisions and chemistry.

SPARTA Direct Simulation Monte Carlo Simulator
The utility and performance of the direct simulation Monte Carlo ray-tracing methods in engineering problems involving realistic properties are examined. Strategies are compared for treating anisotropic scattering distributions, nonuniform temperatures and radiative properties, and spectral property variations.

Monte Carlo Analysis - an overview | ScienceDirect Topics
Monte Carlo simulations are applied to many topics including quantum chromodynamics, cancer radiation therapy, traffic flow, stellar evolution and VLSI design. All these simulations require the use of random numbers and therefore pseudorandom number generators, which makes creating random-like numbers very important. A simple example of how a computer would perform a Monte Carlo simulation is the calculation of π. If a square enclosed a circle and a point were randomly chosen inside the ...

Monte Carlo method - Wikipedia
PURPOSE: Monte Carlo (MC) track structure codes are commonly used for predicting energy deposition and radiation-induced DNA damage at the nanometer scale. Various simulation parameters such as physics model, DNA model, and direct damage threshold have been developed.

Monte Carlo simulations of energy deposition and DNA ...
Abstract. Abstract The principles of and procedures for implementing direct simulation Monte Carlo (DSMC) are described. Guidelines to inherent and external errors common in DSMC applications are provided. Three applications of DSMC to transitional and nonequilibrium flows are considered: rarefied atmospheric flows, growth of thin films, and microsystems.

DIRECT SIMULATION MONTE CARLO: Recent Advances and ...
Direct simulation Monte Carlo on petaflop supercomputers and beyond Physics of Fluids, Vol. 31, No. 8 Combining particle-in-cell and direct simulation Monte Carlo for the simulation of reactive plasma flows Physics of Fluids, Vol. 31, No. 7

Direct Simulation Monte Carlo Simulations of Hypersonic ...
In this paper, the basic ideas underlying the Direct Simulation Monte Carlo (DSMC) method are examined and a novel nonhomogeneous N-particle kinetic equation describing the randomized mathematical model of DSMC is derived.

On the basic concepts of the direct simulation Monte Carlo ...
The proposed Monte Carlo simulation approach is built with four customizable parameters: Basic Reproduction Number (a measure of rate of transmission, R0), Infection Fatality Rate (IFR), Weeks from...

*Monte Carlo Simulations to Democratize COVID-19 Policies**
S.N. Chakraborty, L.D. GelbA Monte Carlo simulation study of methane clathrate hydrates confined in slit-shaped pores J. Phys. Chem. B, 116 (2012), pp. 2183-2197 Google Scholar

Monte Carlo simulation studies of clathrate hydrates: A ...
Monte-Carlo simulations simply mean perform your simulation with varying inputs such that the inputs are chosen randomly. Better MC simulations use prior information / simulations to pick the next iteration. Here is an example - given an input, the method passes if it is greater than 0.5, fails if it is less than or equal to 0.5.

How to write a Monte Carlo Simulation Code? - MATLAB ...
Monte Carlo simulation is a technique that was developed by both Neumann and

Stanislaw Ulam to help individuals determine the level of risk and help with decision making. The Monte Carlo simulation technique helps a ton of professionals in different sectors.

How Monte Carlo Simulation Works? - Management Study HQ

Monte Carlo simulation brings insight into these kinds of uncertainties. This course will introduce you to Monte Carlo Simulation using Microsoft excels built in statistical functions to get started. You just need Native Excel in this course. Here's what you'll learn.

Monte Carlo Simulation Fundamentals | Pluralsight

Monte Carlo Simulation Now that the data has been appropriately transformed, a Monte Carlo simulation is generated to analyse the potential range of outcomes for page view statistics. The page views are expressed in logarithmic format, in accordance with the chosen distribution.

This thesis develops and evaluates Gap-tooth DSMC (GT-DSMC), a direct Monte Carlo simulation procedure for dilute gases combined with the Gap-tooth method of Gear, Li, and Kevrekidis. The latter was proposed as a means of reducing the computational cost of microscopic (e.g. molecular) simulation methods using simulation particles only in small regions of space (teeth) surrounded by (ideally) large gaps. This scheme requires an algorithm for transporting particles between teeth. Such an algorithm can be readily developed and implemented within direct Monte Carlo simulations of dilute gases due to the non-interacting nature of the particle-simulators. The present work develops and evaluates particle treatment at the boundaries associated with diffuse-wall boundary conditions and investigates the drawbacks associated with GT-DSMC implementations which detract from the theoretically large computational benefit associated with this algorithm (the cost reduction is linear in the gap-to-tooth ratio). Particular attention is paid to the additional numerical error introduced by the gap-tooth algorithm as well as the additional statistical uncertainty introduced by the smaller number of particles. We find the numerical error introduced by transporting particles to adjacent teeth to be considerable. Moreover, we find that due to the reduced number of particles in the simulation domain, correlations persist longer, and thus statistical uncertainties are larger than DSMC for the same number of particles per cell. This considerably reduces the computational benefit associated with the GT-DSMC algorithm. We conclude that the GT-DSMC method requires more development, particularly in the area of error and uncertainty reduction, before it can be used as an effective simulation method.

Direct Simulation Monte Carlo is a well-established method for the computer simulation of a gas flow at the molecular level. While there is a limit to the size of the flow-field with respect to the molecular mean free path, personal computers now allow solutions well into the continuum flow regime. The method can be applied to basic problems in gas dynamics and practical applications range from microelectromechanics systems (MEMS) to astrophysical flows. DSMC calculations have assisted in the design of vacuum systems, including those for semiconductor manufacture, and of many space vehicles and missions. The method was introduced

by the author fifty years ago and it has been the subject of two monographs that have been published by Oxford University Press. It is now twenty years since the second of these was written and, since that time, most DSMC procedures have been superseded or significantly modified. In addition, visual interactive DSMC application programs have been developed that have proved to be readily applicable by non-specialists to a wide variety of practical problems. The computational variables are set automatically within the code and the programs report whether or not the criteria for a good calculation have been met. This book is concerned with the theory behind the current DSMC molecular models and procedures, with their integration into general purpose programs, and with the validation and demonstration of these programs. The DSMC and associated programs, including all source codes, can be freely downloaded through links that are provided in the book. The main accompanying program is simply called the "DSMC program" and, in future versions of the book, it will be applicable to homogeneous (or zero-dimensional) flows through to three-dimensional flow. All DSMC simulations are time-accurate unsteady calculations, but the flow may become steady at large times. The current version of the DSMC code is applicable only to zero and one-dimensional flows and the older DS2V code is employed for the two-dimensional validation and demonstration cases. It is because of this temporary use of the older and well-proven program that the DS2V source code is made freely available for the first time. Most of the homogeneous flow cases are validation studies, but include internal mode relaxation studies and spontaneous and forced ignition leading to combustion in an oxygen-hydrogen mixture. The one-dimensional cases include the structure of a re-entry shock wave that takes into account electronic excitation as well as dissociation, recombination and exchange reactions. They also include a spherically imploding shock wave and a spherical blast wave. The two-dimensional and axially-symmetric demonstration cases range from a typical MEMS flow to aspects of the flow around rotating planets. Intermediate cases include the formation and structure of a combustion wave, a vacuum pump driven by thermal creep, a typical vacuum processing chamber, and the flow around a typical re-entry vehicle

"The book is divided into two parts based on the overall goals, with the first part focusing on fundamental considerations, and the second part dedicated to describing computer simulation methods. The first section covers three different areas: (1) kinetic theory, (2) quantum mechanics, and (3) statistical mechanics. Important results from these three areas are then brought together to allow analysis of nonequilibrium processes in a gas based on molecular level considerations. Chapter 1 covers kinetic theory, in which the basic idea is to develop techniques to relate the properties and behavior of particles, representing atoms and molecules, to the fluid mechanical aspects of a gas at the macroscopic level. This requires us to provide a basic definition by what is meant by a particle, and how these particles interact with one another through the mechanism of inter-molecular collisions. This leads us into a discussion of modeling of macroscopic molecular transport processes, such as viscosity and thermal conductivity, that represents one of the first key successes of kinetic theory. We will find that kinetic theory relies on the use of statistical analysis techniques, such as probability density functions, due to the very large volumes of information involved in tracking the behavior of every single particle in a real gas flow"--

The prediction of rocket nozzle internal and external flowfields is an important aspect

of space system design analysis, particularly with regard to exhaust plume contamination potential in the backflow region. For small engine plumes expanding into vacuum, the rarefied nonequilibrium effects both inside and outside of the nozzle render the conventional continuum method of analysis invalid in principle. To properly assess the backflow contamination flux due to inter-molecular collisions, molecular simulation of the flowfields is necessary. The objective of the present work is to subject such a simulation method to the scrutiny of a direct comparison with data taken from a simulated vacuum expansion of a 22.24N (51bf) rocket nozzle. The results of the successful application of the Direct Simulation Monte Carlo (DSMC) method to predict the mass flux density in the plume of a bipropellant engine are presented. The entire flow field starting from the nozzle throat extending to the backflow region has been calculated. Parameters varied in the simulation study include the nozzle area ratio and the internal degrees of freedom of the gas mixture. The results from DSMC calculation for all cases exhibit the same magnitude and behavior as the experimental data within expected statistical scatter. The angular mass fluxes in the backflow region are nearly independent of the parameters examined.

This monograph surveys the present state of Monte Carlo methods. we have dallied with certain topics that have interested us Although personally, we hope that our coverage of the subject is reasonably complete; at least we believe that this book and the references in it come near to exhausting the present range of the subject. On the other hand, there are many loose ends; for example we mention various ideas for variance reduction that have never been seriously appli(:d in practice. This is inevitable, and typical of a subject that has remained in its infancy for twenty years or more. We are convinced Qf:ver theless that Monte Carlo methods will one day reach an impressive maturity. The main theoretical content of this book is in Chapter 5; some readers may like to begin with this chapter, referring back to Chapters 2 and 3 when necessary. Chapters 7 to 12 deal with applications of the Monte Carlo method in various fields, and can be read in any order. For the sake of completeness, we cast a very brief glance in Chapter 4 at the direct simulation used in industrial and operational research, where the very simplest Monte Carlo techniques are usually sufficient. We assume that the reader has what might roughly be described as a 'graduate' knowledge of mathematics. The actual mathematical techniques are, with few exceptions, quite elementary, but we have freely used vectors, matrices, and similar mathematical language for the sake of conciseness.

Over the past several decades, atomic oxygen (AO) measurements taken from sounding rocket sensor payloads in the Mesosphere and lower Thermosphere (MALT) have shown marked variability. AO data retrieved from the second Coupling of Dynamics and Aurora (CODA II) experiment has shown that the data is highly dependent upon rocket orientation. Many sounding rocket payloads, including CODA II, contain AO sensors that are located in close proximity to the payload surface and are thus significantly influenced by compressible, aerodynamic effects. In addition, other external effects such as Doppler shift and the contamination of sensor optics from desorption may play a significant role. These effects serve to inhibit the AO sensors' ability to accurately determine undisturbed atmospheric conditions. The present research numerically models the influence caused by these effects (primarily

aerodynamic), using the direct simulation Monte Carlo (DSMC) method. In particular, a new parallel, steady/unsteady, three-dimensional, DSMC solver, foamDSMC, is developed. The method of development and validation of this new solver is presented with comparisons made with available commercial solvers. The foamDSMC solver is then used to simulate the steady and unsteady flow-field of CODA II, with steady-state simulations conducted along 2 km intervals and unsteady simulations conducted near apogee. The results based on the compressible flow aerodynamics as well as Doppler shift and contamination effects are all examined, and are used to create correction functions based on the ratio of undisturbed to disturbed flowfield concentrations. The numerical simulations verify the experimental results showing the strong influence of rocket orientation on concentration, and show conclusive evidence pointing to the success of the correction functions to significantly minimize the external effects previously mentioned. In addition to the correction function approach, the optimal placement of the AO sensor along the sounding rocket fuselage is addressed as well as results pertaining to "shock-freeze" simulations.

This accessible new edition explores the major topics in Monte Carlo simulation that have arisen over the past 30 years and presents a sound foundation for problem solving Simulation and the Monte Carlo Method, Third Edition reflects the latest developments in the field and presents a fully updated and comprehensive account of the state-of-the-art theory, methods and applications that have emerged in Monte Carlo simulation since the publication of the classic First Edition over more than a quarter of a century ago. While maintaining its accessible and intuitive approach, this revised edition features a wealth of up-to-date information that facilitates a deeper understanding of problem solving across a wide array of subject areas, such as engineering, statistics, computer science, mathematics, and the physical and life sciences. The book begins with a modernized introduction that addresses the basic concepts of probability, Markov processes, and convex optimization. Subsequent chapters discuss the dramatic changes that have occurred in the field of the Monte Carlo method, with coverage of many modern topics including: Markov Chain Monte Carlo, variance reduction techniques such as importance (re-)sampling, and the transform likelihood ratio method, the score function method for sensitivity analysis, the stochastic approximation method and the stochastic counter-part method for Monte Carlo optimization, the cross-entropy method for rare events estimation and combinatorial optimization, and application of Monte Carlo techniques for counting problems. An extensive range of exercises is provided at the end of each chapter, as well as a generous sampling of applied examples. The Third Edition features a new chapter on the highly versatile splitting method, with applications to rare-event estimation, counting, sampling, and optimization. A second new chapter introduces the stochastic enumeration method, which is a new fast sequential Monte Carlo method for tree search. In addition, the Third Edition features new material on: • Random number generation, including multiple-recursive generators and the Mersenne Twister • Simulation of Gaussian processes, Brownian motion, and diffusion processes • Multilevel Monte Carlo method • New enhancements of the cross-entropy (CE) method, including the "improved" CE method, which uses sampling from the zero-variance distribution to find the optimal importance sampling parameters • Over 100 algorithms in modern pseudo code with flow control • Over 25 new exercises Simulation and the Monte Carlo Method, Third Edition is an excellent text for upper-undergraduate and beginning graduate courses in stochastic simulation and Monte Carlo techniques. The book also serves as a valuable reference

for professionals who would like to achieve a more formal understanding of the Monte Carlo method. Reuven Y. Rubinstein, DSc, was Professor Emeritus in the Faculty of Industrial Engineering and Management at Technion-Israel Institute of Technology. He served as a consultant at numerous large-scale organizations, such as IBM, Motorola, and NEC. The author of over 100 articles and six books, Dr. Rubinstein was also the inventor of the popular score-function method in simulation analysis and generic cross-entropy methods for combinatorial optimization and counting. Dirk P. Kroese, PhD, is a Professor of Mathematics and Statistics in the School of Mathematics and Physics of The University of Queensland, Australia. He has published over 100 articles and four books in a wide range of areas in applied probability and statistics, including Monte Carlo methods, cross-entropy, randomized algorithms, tele-traffic c theory, reliability, computational statistics, applied probability, and stochastic modeling.

The direct simulation Monte Carlo method has been extended to describe the detailed chemistry in the ionosphere. A theoretical relationship between the continuum reaction rates and the reaction cross sections required for the Monte Carlo simulation has been established. The effects of high energy electrons on the ambient ionosphere has been investigated and details of the nonequilibrium results are presented. (Author).